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Title: xRage: Setting ambient region state

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# xRage: Setting ambient region state

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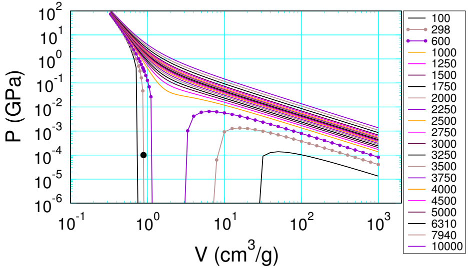
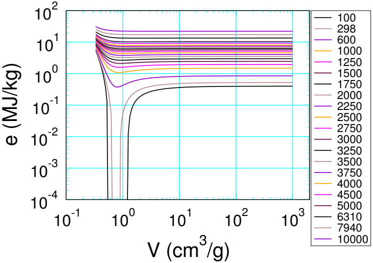
# Sesame table

Equation of state (EOS)

- Independent thermodynamic variables: $\rho$ and $T$
- Tables for $P(\rho, T)$ and $e(\rho, T)$

<u>Example</u>: Nitromethane isotherms (log-log scale to cover wide domain)




Phase space of interest for detonation wave simulation $P > 0.1$ GPa

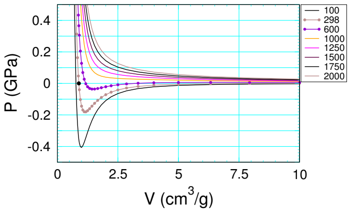
Issue at ambient state: 1 bar and 298 K, despite point in table

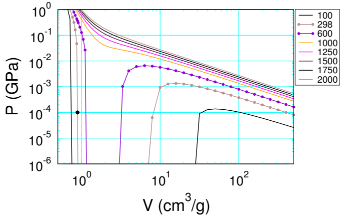
# van der Waal loop

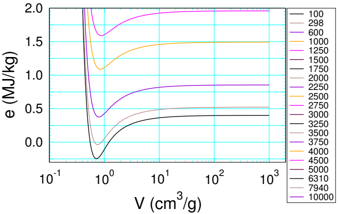
Compressibility $K_T = -V(\partial_V P)_T > 0$ required for thermodynamic stability

$K_s = K_T + \Gamma^2(C_V T/V) > 0$ required for thermodynamic consistency

required for hydro PDEs to be hyperbolic (non-linear wave equations)



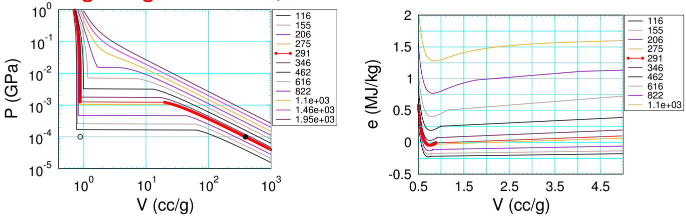
# Maxwell construction and mixed region

xRage generates teos table: $P$, $T$ independent variables

Facilitates PT equilibrium for mixed cell (default hydro)

Unique PT solution only if component EOS are consistent & stable

By default xRage regularizes $K_T < 0$ with Maxwell construction




Horizontal lines in P plot define mixed liquid-vapor region

Small liquid drops surrounded by vapor or phase separated liquid & vapor

Initialization issue

T=298 K isotherm has $P \approx 10^{-3}$ GPa or 10 bar

EOS density at ambient state, $\rho < 0.01$ g/cc (vapor region)

Liquid NM at ambient state has $\rho = 1.125$ g/cc

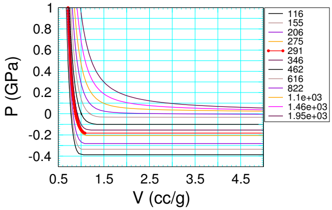
# Comments on EOS

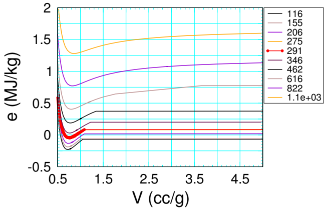
- Even though ambient density not as intended
  Not coding error
- Issue is with nitromethane table
  Peak pressure on van der Waal loop is too high
    With Maxwell construction EOS is qualitatively correct
    But quantitatively inaccurate at low pressures
  High pressure regime not affected by Maxwell construction
- Limited data to calibrate EOS
  Data for shock compression
  Fitting form extrapolated to expansion
    Extrapolations can be quantitatively inaccurate

# Work around

`support_tension = .true.`

Instead of Maxwell construction,
isotherm extended at minimum pressure on van der Waal loop




Next issue:

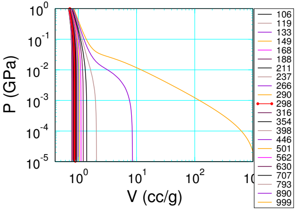
Nearest isotherm to 298 K room temperature is $T = 291$ K
Interpolated density slightly off (depends on teos grid spacing)
even though sesame table has isotherm at 298 K

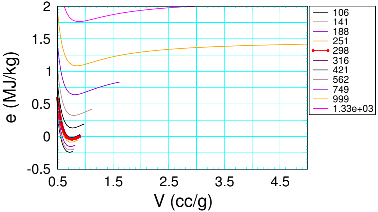
# Adjust teos grid

Set teos.in input `tevlo,tevhi,numtevdec` such that

`tevlo = T0 * 10**(-j/numtevdec)` for some integer `j`

and similarly for `P0`




Then for xRage input

`tevreg=T0` and `prsreg=P0`

get value of density from point on sesame table

# Comment on interpolation

- Sesame table to teos table
  Independent variables $(V, T) \leftrightarrow (P, T)$
  1 to 1 iff $P(V)$ monotonic on all isotherms ($K_T > 0$)
  In mixed region $P$ is constant on isotherm and $V$ not unique
  Mixed cell EOS equations ($P$-$T$ equilibrium) can be stiff
- Accuracy of interpolation
  Depends on smoothness of function relative to $(P, T)$ grid
  Logarithmic grid spacing increases accuracy for large $P$
  but not helpful in mixed region with support tension
  `numprsdec,numtevdec` sets grid size
  but accuracy can be limited by coarse grid on sesame table
- Derivatives (such as sound speed)
  On grid lines, normal derivative is discontinuous